LM-06K137
November 15, 2006

Estimation Uncertainty in the Determination of the Master Curve Reference Temperature

TL Sham and DR Eno

Estimation Uncertainty in the Determination of the Master Curve Reference Temperature

T.L. Sham and D.R. Eno*

Lockheed Martin Corporation
P.O. Box 1072
Schenectady, New York 12301
USA

Abstract

The Master Curve Reference Temperature, T_0, characterizes the fracture performance of structural steels in the ductile-to-brittle transition region. For a given material, this reference temperature is estimated via fracture toughness testing. A methodology is presented to compute the standard error of an estimated T_0 value from a finite sample of toughness data, in a unified manner for both constant temperature and multiple temperature test methods. Using the asymptotic properties of maximum likelihood estimators, closed-form expressions for the standard error of the estimate of T_0 are presented for both test methods. This methodology includes statistically rigorous treatment of censored data, which represents an advance over the current ASTM E1921 methodology. Through Monte Carlo simulations of realistic constant temperature and multiple temperature test plans, the recommended likelihood-based procedure is shown to provide better statistical performance than the methods in the ASTM E1920 standards.

* Correspondence to D.R. Eno, enodr@kapl.gov

Introduction

The prediction of cleavage fracture performance of pressure vessel steels in the ductile-brittle transition region has been extensively investigated. Due to the statistical nature of the cleavage initiation mechanism [1], there is significant scatter in the test data. The data scatter was quantified by Wallin [2] using Weibull statistics. This led to the use of a reference temperature, T_0, in the so-called Master Curve approach to characterize the cleavage fracture performance of a given heat of steel [3]. The test method for the determination of T_0 for uniform material was codified in the ASTM E1921 test standards. The technical basis for the Master Curve approach and the ASTM E1921 standards was documented by Merkle et al. [4].

The ASTM E1921 standards provide the test methods for determining T_0 using a small number of fracture toughness test specimens (6 to 8 specimens). The test method specified in E1921-97 was based on constant temperature testing and a margin adjustment in T_0 was given to cover the estimation uncertainty due to the use of a small sample size. A multiple temperature test method to determine T_0 was added as an option in the E1921-02 edition. In the E1921-05 edition, a method to determine the estimation uncertainty due to finite sample size for both constant temperature and multiple temperature test methods was added.

The standard error of the estimate of T_0, which depends on the difference between test temperature and T_0, is inversely proportional to the square root of the number of valid data used to obtain the estimate. In the E1921 standards, the constant of proportionality is represented as a piecewise constant function of the size-adjusted median fracture toughness, and values of this constant of proportionality are presented in tabulated form.

Engineering approaches have been proposed to extend the constant temperature procedure in evaluating the standard error of the estimate of T_0, to data obtained from the multiple temperature test method. These approaches have been based on defining a surrogate for the median fracture toughness value from a multi-temperature test, then using this value in the single-temperature procedure. One proposal was to define the equivalent median fracture toughness as the average of the median fracture toughness values at different test temperatures [5]. An analogous approach, attributed to Tregoning in [5], was to obtain an equivalent median fracture toughness using the average of the test temperatures. The Reference [5] approach had been recently incorporated into the ASTM E1921-05 standard for multiple temperature tests.

It is shown in this work that standard errors on T_0 for both constant and multiple temperature test methods can be formulated in a statistically rigorous and unified manner. Based on the asymptotic properties of maximum likelihood estimators, the standard error of the estimate on T_0 can be computed using closed-form expressions for both test methods. Data censoring is included in a statistically rigorous manner in the formulation; this represents an advance over the current ASTM E1921-05 standard formulation adapted from Reference [5].

Weibull Description

Consider a pressure vessel steel in a certain material condition (e.g., quenched and tempered, stress relieved, thermally embrittled and/or irradiated). At a given temperature in the ductile-brittle transition region, the fracture toughness values, K , for test specimens (e.g., compact tension specimens) with thickness B follow a three-parameter Weibull distribution [4]. The cumulative distribution function for K is

$$F(K;\ b,\ K_0,\ K_{min}) = 1 - S(K;\ b,\ K_0,\ K_{min}) \quad , \tag{1}$$

where $S(K)$ is the survival probability given by

$$S(K;\ b,\ K_0,\ K_{min}) = exp\left(-\frac{B}{B_0}\left(\frac{K - K_{min}}{K_0 - K_{min}} \right)^b \right) \quad . \tag{2}$$

The parameters b, K_0, and K_{min} are the Weibull parameters. The shape parameter b characterizes the data scatter and the threshold parameter K_{min} specifies the minimum toughness. The parameter K_0 represents the $1-e^{-1}$ quantile (0.623 quantile) of fracture toughness values for test specimens of reference thickness B_0.

The cumulative distribution function, eqn. (1), accounts for the observed specimen size effect on fracture toughness in the ductile-brittle transition region. Given a fracture toughness value of K_1 for a specimen with a thickness B_1, a size-adjusted fracture toughness value, K_2, for a specimen with a thickness B_2 can be determined from

$$K_2 = K_{min} + \left(\frac{B_1}{B_2}\right)^{1/b} \left(K_1 - K_{min}\right) \quad , \tag{3}$$

where the value of the cumulative distribution function for the pair $\left(K_2,\ B_2\right)$ would be the same as that for $\left(K_1,\ B_1\right)$.

Let $K_{(x)}$ represent the x quantile of fracture toughness values for test specimens of thickness B. Then $K_{(x)}$ can be related to K_0 through eqns. (1) and (2) as

$$K_{(x)} - K_{min} = \left(\frac{B_0}{B}\ ln\left(\frac{1}{1-x}\right)\right)^{1/b} \left(K_0 - K_{min}\right) \quad . \tag{4}$$

As a special case, $K_{(0.5)}^{B_0}$, the 0.5 quantile (median) of fracture toughness values for test specimens of thickness $B = B_0$, is given by

$$K_{(0.5)}^{B_0} = K_{min} + \left(ln2\right)^{1/b} \left(K_0 - K_{min}\right) \quad . \tag{5}$$

The temperature trend of the median fracture toughness values for test specimens of thickness $B = B_0$ can be described by

$$K^{B_0}_{(0.5)} = A + D\ exp\left(C\left[T - T_0\right]\right)\ , \tag{6}$$

where A, D and C are empirical curve-fitting parameters, T is the temperature, and T_0 is a reference temperature (or an indexing temperature) that characterizes the fracture performance of the pressure vessel steel in the given material condition. Thus K_0 can be related to T and T_0 through eqns. (5) and (6).

The probability density function $f\left(K\right)$ can be derived from the cumulative distribution function, $F\left(K\right)$, as

$$f\left(K\right) = \frac{dF}{dK} = b\ \frac{B}{B_0}\ \frac{\left(K - K_{min}\right)^{b-1}}{\left(K_0 - K_{min}\right)^{b}}\ exp\left(-\frac{B}{B_0}\left(\frac{K - K_{min}}{K_0 - K_{min}}\right)^{b}\right)\ . \tag{7}$$

Maximum Likelihood Estimation of Reference Temperature and Estimation Uncertainty

Consider fracture toughness tests in the ductile-brittle transition region, using N specimens. Let K_i, T_i and B_i be the fracture toughness value, the test temperature, and the specimen thickness for the i^{th} test, respectively. Test data are considered invalid when either the K-measurement capacity of the specimen size is exceeded, or too much stable crack growth has taken place before cleavage fracture occurs. An invalid fracture toughness datum is censored by replacing the measured fracture toughness value by an appropriately chosen limit. Detailed discussion of fracture toughness data censoring is given in the ASTM E1921-02 and 05 test standards.

Introduce a parameter δ_i for the i^{th} test. It is assigned a value of one when the datum is valid, and zero when the datum is censored. Further, K_i will now denote either the measured or the censored fracture toughness value, as appropriate, for the i^{th} test.

A likelihood function, $\mathcal{L}$, can be defined as [6]

$$\mathcal{L} = \prod_{i=1}^{N} \left[f\left(K_i\right) \right]^{\delta_i} \left[S\left(K_i\right) \right]^{1-\delta_i} \quad , \tag{8}$$

and upon using eqns. (2) and (7), $\mathcal{L}$ takes the form

$$\mathcal{L} = \prod_{i=1}^{N} \left(b\frac{B_i}{B_0} \right)^{\delta_i} \frac{\left(K_i - K_{min}\right)^{(b-1)\delta_i}}{\left(\left(K_0\right)_i - K_{min}\right)^{b\delta_i}} exp\left(-\frac{B_i}{B_0} \left(\frac{K_i - K_{min}}{\left(K_0\right)_i - K_{min}} \right)^b \right) \; , \tag{9}$$

where $\left(K_0\right)_i$ corresponds to K_0 at temperature T_i.

Taking the natural logarithm, the products in eqn. (9) can be converted to sums as

$$\Omega \equiv ln\,\mathcal{L} = \sum_{i=1}^{N} \left(\begin{array}{l} \delta_i\, ln\left(b\dfrac{B_i}{B_0} \right) + \left(b-1\right)\delta_i\, ln\left(K_i - K_{min}\right) \\ -\, b\delta_i\, ln\left(\left(K_0\right)_i - K_{min}\right) - \dfrac{B_i}{B_0}\left(\dfrac{K_i - K_{min}}{\left(K_0\right)_i - K_{min}} \right)^b \end{array} \right) \tag{10}$$

where Ω is referred to as the log-likelihood function.

Using eqns. (5) and (6), $\left(K_0\right)_i - K_{min}$ can be related to the temperature trend as

$$\left(K_0\right)_i - K_{min} = \frac{1}{\left(ln\,2\right)^{1/b}} \left[\left(A - K_{min}\right) + D\;\; exp\left(C\left(T_i - T_0\right)\right) \right] \; . \tag{11}$$

Thus, for prescribed values of the Weibull parameters and the parameters A, D and C in the temperature trend, and a set of fracture toughness data, the log-likelihood function can be treated as a function of the reference temperature T_0, i.e., $\Omega = \Omega(T_0)$.

The reference temperature T_0 can be estimated by maximizing the log-likelihood function with respect to T_0 [6],

$$\frac{\partial \Omega(T_0)}{\partial T_0} = 0 \quad . \tag{12}$$

This leads to a nonlinear algebraic equation for T_0:

$$\begin{aligned}&\sum_{i=1}^{N} \delta_i \frac{exp\left(C\left(T_i - T_0\right)\right)}{\left(\frac{1}{ln\,2}\right)^{1/b}\left[\left(A - K_{min}\right) + D\,exp\left(C\left(T_i - T_0\right)\right)\right]} \\ &- \sum_{i=1}^{N} \frac{exp\left(C\left(T_i - T_0\right)\right)}{\left(\left(\frac{1}{ln\,2}\right)^{1/b}\left[\left(A - K_{min}\right) + D\,exp\left(C\left(T_i - T_0\right)\right)\right]\right)^{b+1}} \left\{\frac{B_i}{B_0}\left(K_i - K_{min}\right)^b\right\} = 0 \quad .\end{aligned} \tag{13}$$

Equation (13) permits the best estimate value of the reference temperature T_0 to be estimated from a finite sample size.

The estimation uncertainty in T_0 can be accounted for in the following manner, based on the asymptotic properties of maximum likelihood estimators. The standard error of the estimation of T_0, σ_{est}, can be estimated as [6]

$$\sigma_{est}^2 = -\left(\frac{\partial^2 \Omega(T_0)}{\partial T_0^2}\right)^{-1} \quad . \tag{14}$$

After some algebraic manipulation, the second derivative of the log-likelihood function can be expressed as

$$\frac{\partial^2 \Omega(T_0)}{\partial T_0^2} = \sum_{i=1}^{N} \delta_i \; P_i + \sum_{i=1}^{N} Q_i \quad , \tag{15}$$

where

$$P_i \equiv - \frac{b \; (A - K_{min}) \; D \; C^{\,2} \, exp\big(C\,(T_i - T_0)\big)}{\big[(A - K_{min}) + D\,exp\big(C\,(T_i - T_0)\big)\big]^{2}} \quad , \tag{16}$$

$$\begin{aligned} Q_i \equiv b \; \frac{B_i}{B_0} \; (ln\,2) \; (K_i - K_{min})^{b} \\ \times \frac{\big[D \; C^{\,2} \, exp\big(C\,(T_i - T_0)\big)\big] \; \big[(A - K_{min}) - b \; D\,exp\big(C\,(T_i - T_0)\big)\big]}{\big[(A - K_{min}) + D\,exp\big(C\,(T_i - T_0)\big)\big]^{b+2}} \quad . \end{aligned} \tag{17}$$

Thus , σ_{est} , can be computed from eqn. (14) using the closed-form expressions in eqns. (15) to (17), once T_0 is found from eqn. (13).

The estimation uncertainty in T_0, denoted as ΔT_0, can be given as

$$\Delta T_0 = Z_{(0.xx)} \; \sigma_{est} \quad , \tag{18}$$

where $Z_{(0.xx)}$ is the $0.xx$ quantile of the standard normal distribution. Thus a margin adjusted T_0 can be obtained from

$$(T_0)_{\text{margin-adjusted}} = \hat{T}_0 + Z_{(0.xx)} \; \sigma_{est} \quad , \tag{19}$$

where $\hat{T}_0$ is the best estimate T_0 value as determined from eqn. (13).

Results for Constant Temperature Tests

The above formulation can be further simplified when the fracture toughness tests are performed at constant temperature. Let $T_i = T$ for all N tests. Equation (13) is now reduced to

$$\left[A - K_{min} + D\,exp\left(C\left(T - T_0\right)\right)\right]^b \left(\sum_{i=1}^{N} \delta_i\right) - \left(ln\,2\right)\sum_{i=1}^{N} \frac{B_i}{B_0}\left(K_i - K_{min}\right)^b = 0 \ . \qquad (20)$$

The reference temperature T_0 can be solved for in closed-form from eqn. (20). The result is

$$T_0 = T - \frac{1}{C}\ ln\left\{ \frac{1}{D} \left(\left(\frac{\left(ln\,2\right)\sum_{i=1}^{N} \frac{B_i}{B_0}\left(K_i - K_{min}\right)^b}{\sum_{i=1}^{N} \delta_i} \right)^{1/b} - \left(A - K_{min}\right) \right) \right\} \ . \qquad (21)$$

Under the condition of constant test temperature, the second derivative of the log-likelihood function, eqn. (15), becomes

$$\begin{aligned} \frac{\partial^2 \Omega\left(T_0\right)}{\partial T_0^2} = & -\frac{b\ \left(A - K_{min}\right)\ D\ C^{\,2}\, exp\left(C\left(T - T_0\right)\right)}{\left[\left(A - K_{min}\right) + D\,exp\left(C\left(T - T_0\right)\right)\right]^{\,2}} \left(\sum_{i=1}^{N} \delta_i\right) \\ & + \frac{\left[b\ D\ C^{\,2}\, exp\left(C\left(T - T_0\right)\right)\right]\left[\left(A - K_{min}\right) - b\ D\,exp\left(C\left(T - T_0\right)\right)\right]}{\left[\left(A - K_{min}\right) + D\,exp\left(C\left(T - T_0\right)\right)\right]^{b+2}} \\ & \times \left(\left(ln\,2\right)\sum_{i=1}^{N} \frac{B_i}{B_0}\left(K_i - K_{min}\right)^b\right) \ , \end{aligned} \qquad (22)$$

Since eqn. (20) must be satisfied by T_0, it can be used to substitute for the second sum on the right hand side of eqn. (22), i.e., the term with sum on K_i, to arrive at

$$\frac{\partial^2 \Omega(T_0)}{\partial T_0^2} = -\left[\frac{b\ D\ C\ \ exp\left(C\left(T-T_0\right)\right)}{\left(A-K_{min}\right)+D\ \ exp\left(C\left(T-T_0\right)\right)}\right]^2\left(\sum_{i=1}^{N}\delta_i\right)\ . \tag{23}$$

Thus the standard deviation, σ_{est}, can be given in closed-form as

$$\sigma_{est} = \frac{\beta}{\sqrt{\sum_{i=1}^{N}\delta_i}}\ , \tag{24}$$

where β has the dimension of temperature and is given by

$$\begin{aligned}\beta &\equiv \frac{\left(A-K_{min}\right)+D\ \ exp\left(C\left(T-T_0\right)\right)}{b\ \mathrm{C}\ D\ \ exp\left(C\left(T-T_0\right)\right)} \\ &= \left[\frac{1}{b\ C}\right]+\left[\frac{A-K_{min}}{b\ \mathrm{C}\ D}\right] exp\left(-C\left(T-T_0\right)\right)\ \ .\end{aligned} \tag{25}$$

It is seen that the parameter β decays exponentially with $T-T_0$. Thus, for a given sample size N, the standard deviation σ_{est} decreases with increasing test temperature in constant temperature tests.

Comparison with ASTM E1921 Standards

The ASTM E1921 standards for the determination of the reference temperature T_0 specify the values of the Weibull parameters b and K_{min}, and the parameters A, C and D for the temperature trend. They are tabulated in Table 1 in both SI and English units. The sum of the parameters A and D is constrained to $100\ MPa\sqrt{m}$ ($91\,ksi\sqrt{in}$). The reference specimen thickness B_0 is set at $25.4\ mm$ (1 inch), which is customarily referred to as 1T.

The 1T-equivalent fracture toughness values are used in the ASTM E1921 procedures for determining T_0. From eqn. (3), the measured and 1T-equivalent fracture toughness values are related by

$$\left(K_i^{1T} - K_{min}\right)^b = B \; \left(K_i - K_{min}\right)^b \quad . \tag{26}$$

Thus, with the values of the parameters as given in Table 1, and B_0 set at 1T, the expression, eqn. (13), for determining T_0 from the multiple temperature test data is the same as that specified in the ASTM E1921-02 and 05 standards. The expression given in eqn. (21) for finding T_0 when the tests are performed under constant temperature condition also reproduces the result given in the E1921 standards.

Using the values of the parameters tabulated in Table 1, the value of β given in eqn. (25) for constant temperature tests is plotted versus the excess temperature $T - T_0$ in Figure 1. The ASTM E1921-02 and 05 standards have placed a restriction on the range of test temperatures and it is given in the form of

$$-50^oC \le T - T_0 \le 50^oC \quad . \tag{27}$$

This valid test temperature range is shown in Figure 1. The value of β from eqn. (25) is 18 at $T - T_0 = -50^oC$ and it decreases to 13.9 at $T - T_0 = 50^oC$. With respect to the test temperature range in the E1921-02 and 05 standards, constant test temperature at the upper limit of $T_0 + 50^oC$ would lead to the most accurate T_0 estimation for a given number of valid data. However, it is noted that it may be more challenging to obtain valid test data in the upper test temperature region due to considerations such as specimen K-measurement capacity or too much stable crack extension before cleavage fracture takes place.

The ASTM E1921 standards also provide estimates of β, but in terms of the 1T median toughness, $K^{1T}_{(0.5)}$, in tabulated form. In order to compare the results from eqn. (25) with the estimates from the E1921 standards, β is rewritten, using eqn. (6), as

$$\beta = \frac{1}{b\ \mathrm{C}} \ \frac{K^{1T}_{(0.5)} - K_{min}}{K^{1T}_{(0.5)} - A} = \frac{1}{b\ \mathrm{C}}\left(1 + \frac{A - K_{min}}{K^{1T}_{(0.5)} - A}\right) \ . \tag{28}$$

Similarly, the E1921 restriction on the test temperature, eqn. (27), can be converted to an equivalent restriction on the 1T median toughness as

$$57\ MPa\sqrt{m} \le \ K^{1T}_{(0.5)} \ \le 211\ MPa\sqrt{m} \ . \tag{29}$$

Figure 2 compares the values of β from eqn. (28) with those tabulated in the E1921-97 and 05 standards. It is seen that the values of β from eqn. (28) are less restrictive than the estimates given in the E1921-97 and 05 standards, and hence would give smaller margin adjustments on T_0.

<u>Finite Sample Performance of the Estimation Uncertainty Estimates</u>

The margin adjustment given by eqn. (19) was derived on the basis of the asymptotic properties of maximum likelihood estimators. This ensures that in the limit as the number of valid tests approaches infinity, the margin adjustment will provide the nominal coverage (e.g., a 95% upper bound on T_0 will, in fact, have a 95 percent probability of bounding the true material T_0 from above). In practice it would typically be of interest to compute only an upper bound on an estimated T_0 value; however, a lower bound on T_0 could be computed as well by subtracting the margin adjustment from the estimated T_0 rather than adding it.

To assess the characteristics of the E1921 standard and likelihood-based margin adjustments for typical small sample sizes that might be used in practice, a simulation study was undertaken.

This entailed repeatedly generating random samples of simulated toughness data (K_i values), using sample sizes ranging from six to twenty-four, then estimating T_0 and upper and lower 95% margin adjusted T_0 values for each simulated data set. The simulated data samples were generated according to the assumed Master Curve model (eqns. (1), (2), (5), and (6)); for simplicity, all specimen sizes were assumed to be 1T. When a simulated K_{Jc} value generated from the assumed Master Curve model exceeded $K_{Jc(\text{limit})}$, the maximum value of the K_{Jc} capacity of the specimen, the simulated datum was censored at $K_{Jc(\text{limit})}$; this was done to incorporate an important type of data censoring from the ASTM E1921 procedure. Each simulation run described subsequently consisted of 10,000 simulated data sets. It is noted that the likelihood-based margin adjustment (eqn. 19) is not inherently restricted to a temperature range of $T_0 - 50$ to $T_0 + 50^oC$. The simulation results presented below for the likelihood-based margin adjustment are based on using all simulated data, without enforcing a restricted temperature range.

For constant temperature testing, the finite sample performance of the likelihood based bounds is summarized in Figure 3. This figure compares the observed coverage levels of 95% upper bounds on T_0, 95% lower bounds on T_0, and the resulting 90% two-sided confidence intervals for T_0, computed via the likelihood-based margin adjustment (i.e., eqn. (19)). Since the size of the margin adjustment depends on test temperature, test temperatures of $T_0 - 50$, T_0, and $T_0 + 50^oC$ were considered. However, the coverage results were similar for all three cases, so Figure 3 displays the overall coverage probabilities (based on a total of 30,000 simulation runs). The results indicate that the observed coverage of the upper bounds slightly exceeds the nominal coverage, while the observed coverage of the lower bounds slightly underperforms relative to nominal coverage. This asymmetry in coverage between the upper and lower bounds is not surprising, since the margin adjustment is based on a normal distribution assumption, which holds only in the asymptotic limit. For both the lower and upper bounds, a tendency to converge to nominal coverage with increasing sample size is observed. The overall coverage approximates the nominal coverage quite closely over all sample sizes.

For the case of multiple temperature testing, toughness data were simulated at temperatures of $T_0 - 50$, $T_0 - 25$, $T_0 + 25$, and $T_0 + 50^o C$. Five sample sizes were considered, corresponding to two, three, four, five, and six specimens per temperature (actual sample sizes of 8, 12, 16, 20, and 24). The results of the assessment for the likelihood-based margin adjustment (eqn. 19) are shown in Figure 4, which has the same format as Figures 3(a) through 3(c). The same trends are evident in the multiple temperature case as were observed in the constant temperature case The results shown in Figures 3 and 4 would not be changed appreciably even if the toughness data were to be simulated at other chosen temperature intervals.

Figure 5 summarizes the results of the simulation study in terms of the average standard error of T_0 as a function of sample size and test design, for the likelihood-based standard error (eqn. 24 – 25). Testing at higher temperatures leads to a smaller standard error on T_0; this is expected, due to the steepness of the median toughness curve at higher temperatures. The performance of the multiple temperature testing is similar to that of constant temperature testing at T_0. However, the multiple temperature test design has the advantage of allowing for assessment of the fit of the Master Curve temperature sensitivity model, which is not afforded by any constant temperature test.

The coverage properties of the E1921-05 standard method for determining a margin adjustment on T_0 were also assessed via simulation. For single temperature designs, test temperatures between $T_0 - 50$ and $T_0 + 50^o C$ were considered, in ten degree increments. The E1921-05 standard method restricts test temperature to be within $50^o C$ of T_0 for all test results. This restriction is mirrored in the margin adjustment table presented in section X4.2 of the E1921-05 standard; however, in that context, the restriction is implicitly enforced through a lower bound on median toughness. When the test temperature is close to $T_0 - 50$ or $T_0 + 50^o C$, the estimation uncertainty in T_0 can have the effect of making the toughness data appear to be further than $50^o C$ from T_0; in this case, the standard method of calculating the margin adjustment does not apply. In the simulation analysis, then, only simulated data sets for which the standard margin adjustment was applicable were retained in computing coverage probabilities.

Figure 6 displays the simulated coverage probabilities for single temperature testing, using the E1921-05 standard margin adjustment, with coverage results for all test temperatures combined; the format is identical to that of Figures 3 and 4. Figure 7 displays corresponding results for multiple temperature testing. It can be observed from Figures 6 and 7 that the E1921-05 method of computing the margin adjustment on T_0 is conservative relative to the nominal confidence level, both for one-sided coverage and two-sided interval coverage. This conservatism is not surprising in light of the comparison illustrated previously in Figure 2. More importantly, the E1921-05 method does not converge to nominal coverage as the sample size increases.

Figure 8 compares the average standard error on T_0 between the likelihood-based method and the E1921-05 standard method, for the case of multiple temperature testing. As expected, the conservative E1921-05 method yields higher standard errors than the likelihood-based method. Although not shown, constant temperature tests demonstrate a similar relationship between the two methods.

Summary

Based on the asymptotic properties of maximum likelihood estimators, closed form expressions for evaluating the standard error of the estimated Master Curve reference temperature T_0 have been developed for both constant temperature and multiple temperature fracture toughness test methods. The likelihood-based approach provides a unified methodology, covering both test methods, and accommodates censored data in a statistically rigorous way. The asymptotic properties of the maximum likelihood method ensure consistent behavior of the estimators as sample size increases.

Monte Carlo simulations have been performed and the results show that the observed coverage is sufficiently close to nominal to warrant the use of the asymptotic margin adjustment of eqn. (19) in practice. The E1921-05 standard method is conservative, providing higher than nominal coverage probability with larger standard errors than the likelihood-based method.

References

1. Smith, E. The nucleation and growth of cleavage microcracks in mild steel. In: *Physical Basis of Yield and Fracture*, 1966, Institute of Physics and Physical Society, London, pp. 36-45.

2. Wallin, K. The scatter in K_{Jc} -results. Engineering Fracture Mechanics, 1984; 19:1085-1093.

3. Wallin, K. Fracture toughness transition curve shape for ferritic structural steels. In: *Fracture of Engineering Materials and Structures*, Eds. Teoh, SH, Lee, KH, 1991, Elsevier Applied Science, London. pp. 83-88.

4. Merkle, JG, Wallin, K, McCabe, DE. Technical basis for an ASTM standard on determining the reference temperature, T_0, for ferritic steels in the transition range. 1998, NUREG/CR-5504, US Nuclear Regulatory Commission.

5. Lucon, E, Scibetta, M, Van Walle, E. Assessment of the master curve approach on three reactor pressure vessel steels. International Journal of Fracture, 2003, 119:161-178.

6. Meeker, WQ, Escobar, LA. *Statistical Methods for Reliability Data*, 1998, Wiley Interscience, New York.

Table Captions

Table 1, Values of the Weibull parameters β and K_{min}, and the parameters A, C, and D that describe the temperature trend of the 1T equivalent median fracture toughness (the Master Curve), per the E1921 standards. The sum of A and D is constrained to $100\ MPa\sqrt{m}$ ($91\ ksi\sqrt{in}$).

Figure Captions

Figure 1, Plot of parameter β $\left(\equiv \sigma_{est} / \sqrt{\sum_{i=1}^{N} \delta_i}\right)$ as a function of the excess temperature, $T - T_0$, for constant temperature fracture toughness tests. The values of β at the upper ($T = T_0 + 50^oC$) and lower ($T = T_0 - 50^oC$) valid test temperatures per E1921-02 standards are 13.9^oC and 18^oC, respectively.

Figure 2, Plot of parameter β versus the 1T equivalent median toughness for constant temperature fracture toughness tests. Horizontal lines represent the β values recommended in the E1921-97 standards.

Figure 3, Plot of the observed coverage levels of (a) 95% upper bounds, (b) 95% lower bounds, and (c) 90% two-sided confidence intervals, for T_0 at different test temperature and sample size. The results are from the Monte Carlo simulations of constant temperature fracture toughness tests, with margins computed via the likelihood-based method (eqn. 19).

Figure 4, Plot of the observed coverage levels of (a) 95% upper bounds, (b) 95% lower bounds, and (c) 90% two-sided confidence intervals, for T_0 at different test temperature and sample size. The results are from the Monte Carlo simulations of multiple temperature fracture toughness tests, with margins computed via the likelihood-based method (eqn. 19).

Figure 5, Summary plot of average standard error (1 standard deviation) of T_0 as a function of sample size obtained from the Monte Carlo simulations of constant temperature and multiple temperature fracture toughness tests.

Figure 6, Plot of the observed coverage levels of (a) 95% upper bounds, (b) 95% lower bounds, and (c) 90% two-sided confidence intervals, for T_0 at different test temperature and sample size. The results are from the Monte Carlo simulations of constant temperature fracture toughness tests, with margins computed via the E1921-05 standard method (eqn. 19).

Figure 7, Plot of the observed coverage levels of (a) 95% upper bounds, (b) 95% lower bounds, and (c) 90% two-sided confidence intervals, for T_0 at different test temperature and sample size. The results are from the Monte Carlo simulations of multiple temperature fracture toughness tests, with margins computed via the E1921-05 standard method method (eqn. 19).

Figure 8, Summary plot of average standard error (1 standard deviation) of T_0 as a function of sample size obtained from the Monte Carlo simulations of multiple temperature fracture toughness tests, for both the likelihood-based method (eqn. 19) and the E1921-05 standard method.

	b	K_{min}	A	D	C
US Customary Units	4	$18.2\ ksi\sqrt{in}$	$27.3\ ksi\sqrt{in}$	$63.7\ ksi\sqrt{in}$	$0.0106\,/^{o}\,F$
SI Units	4	$20\ MPa\sqrt{m}$	$30\ MPa\sqrt{m}$	$70\ MPa\sqrt{m}$	$0.019\,/^{o}\,C$

Table 1

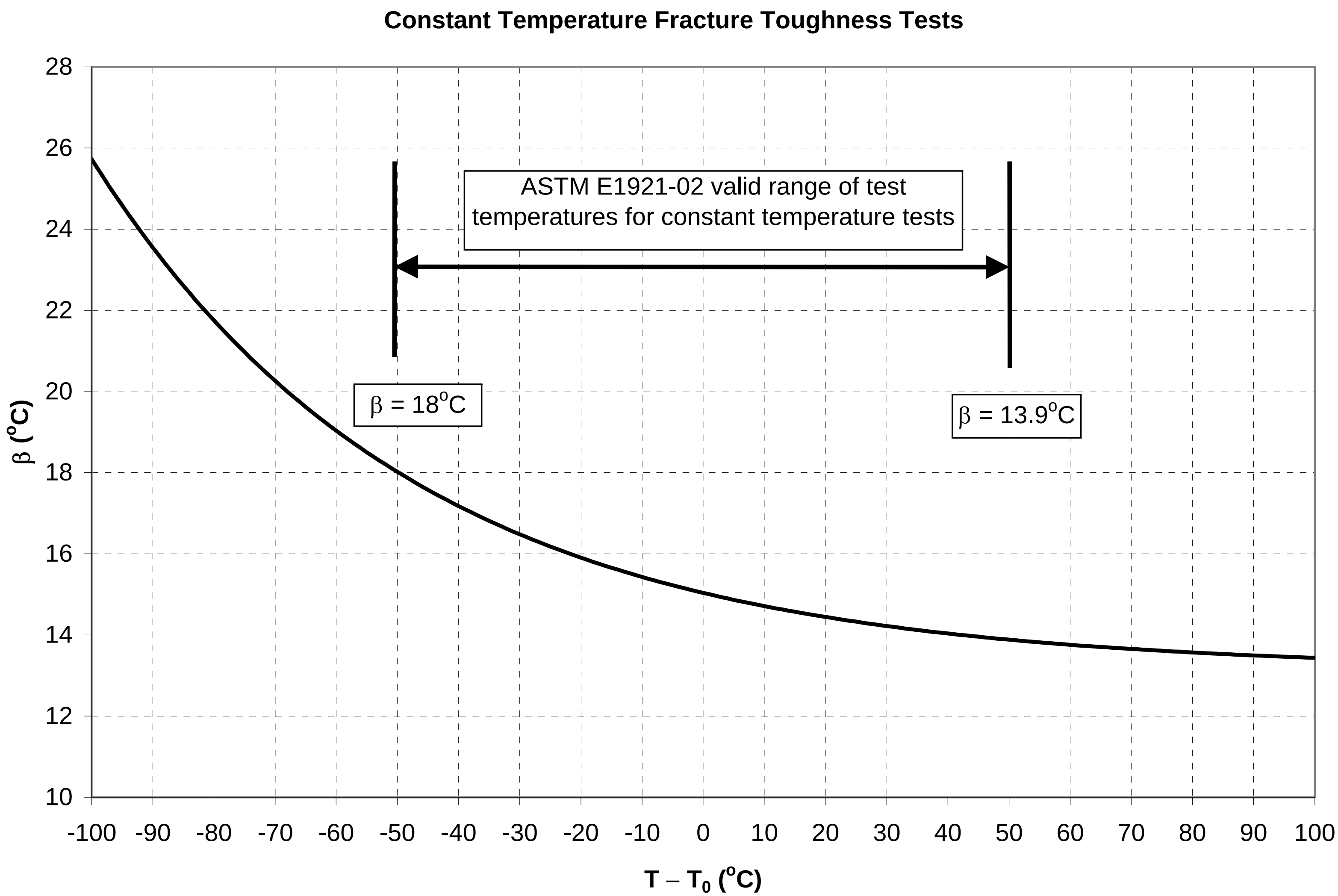

Constant Temperature Fracture Toughness Tests
ASTM E1921-02 valid range of test temperatures for constant temperature tests
β = 18°C
β = 13.9°C
β (°C)
T – T0 (°C)
28
26
24
22
20
18
16
14
12
10
-100
-90
-80
-70
-60
-50
-40
-30
-20
-10
0
10
20
30
40
50
60
70
80
90
100

Figure 1

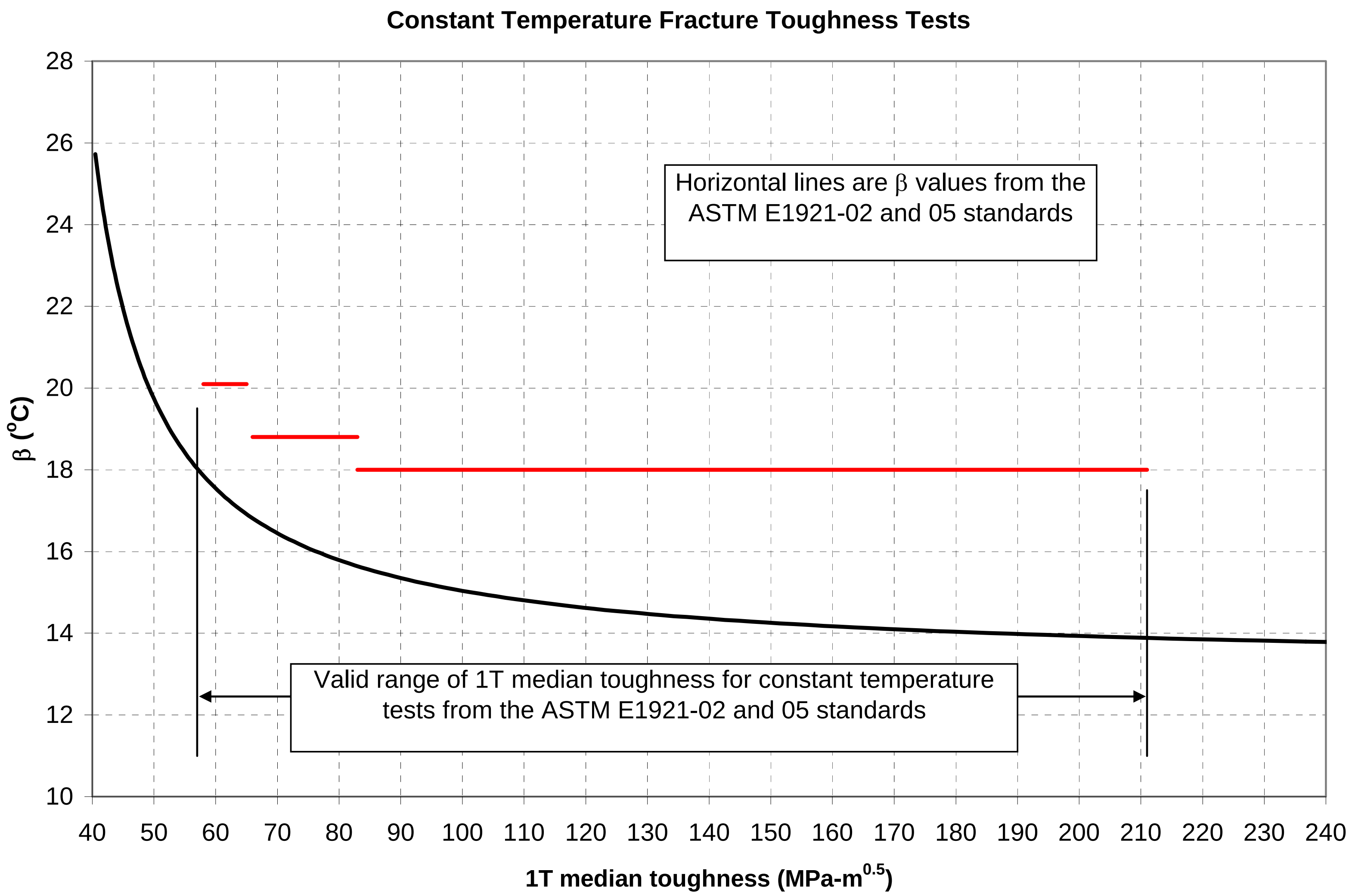
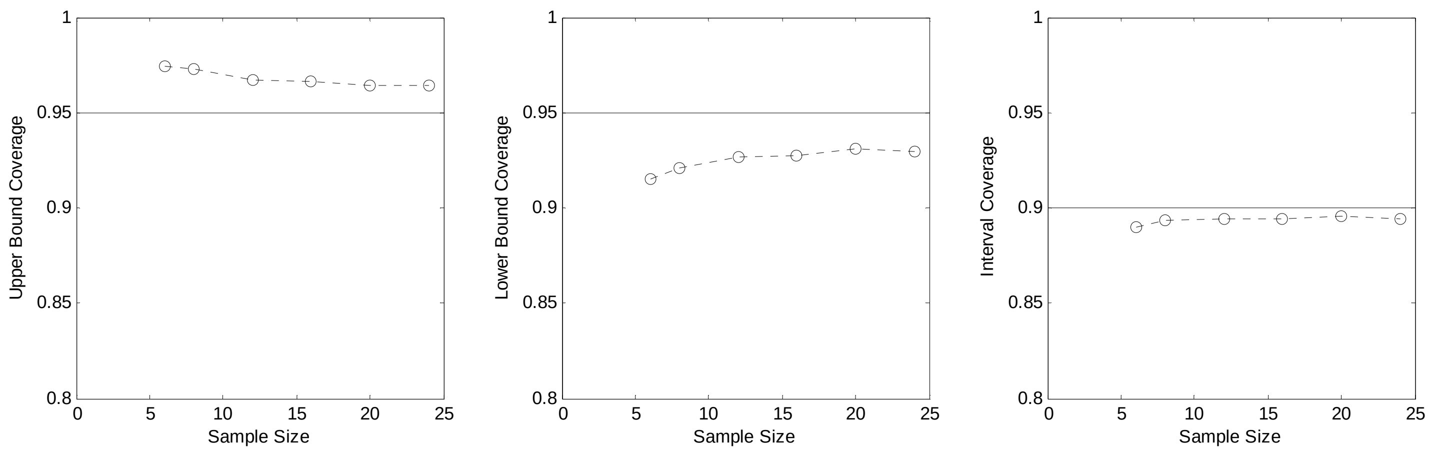

Constant Temperature Fracture Toughness Tests
28
26
24
22
20
18
16
14
12
10
β (ºC)
Horizontal lines are β values from the ASTM E1921-02 and 05 standards
Valid range of 1T median toughness for constant temperature tests from the ASTM E1921-02 and 05 standards
40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240
1T median toughness (MPa-m0.5)

Figure 2


Upper Bound Coverage
Lower Bound Coverage
Interval Coverage
Sample Size
1
0.95
0.9
0.85
0.8
0
5
10
15
20
25

(a) (b) (c)

Figure 3

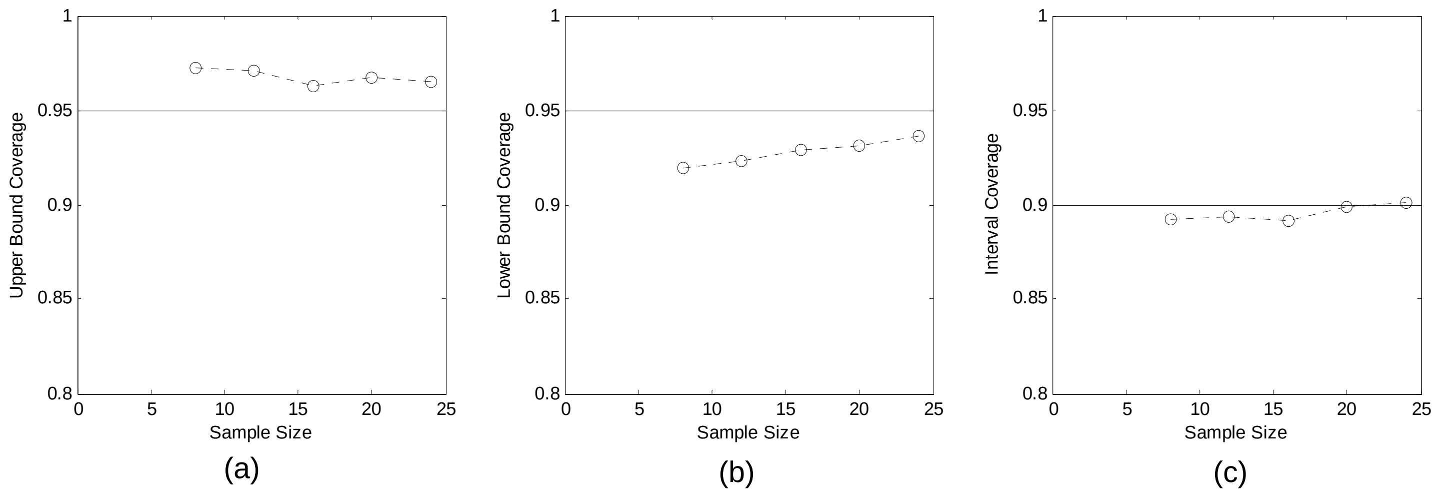
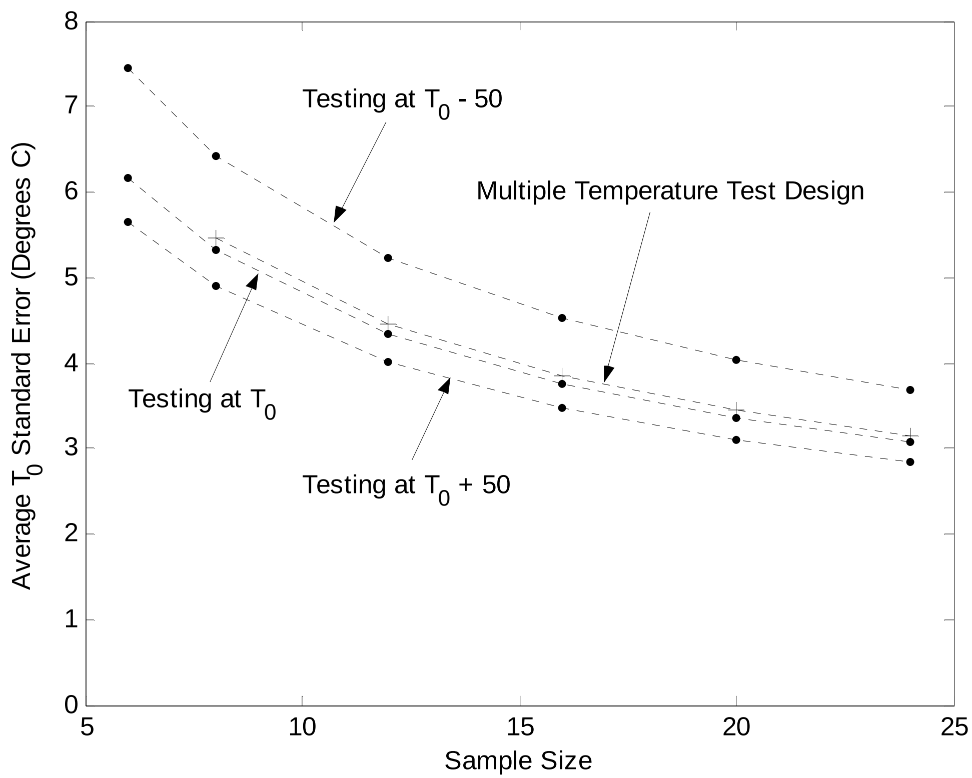
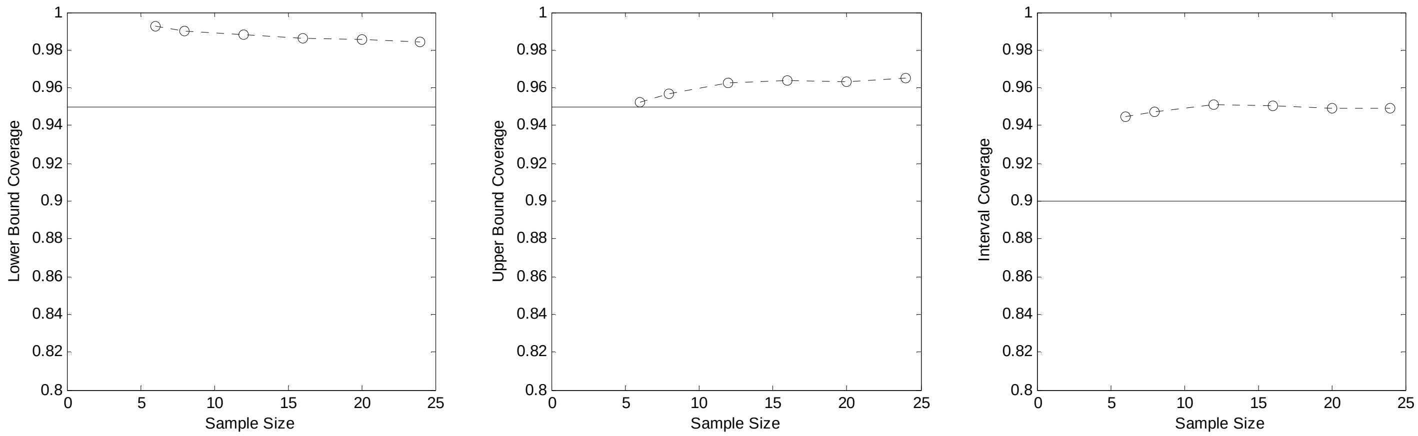

Upper Bound Coverage
Sample Size
(a)
Lower Bound Coverage
Sample Size
(b)
Interval Coverage
Sample Size
(c)
1
0.95
0.9
0.85
0.8
0
5
10
15
20
25

Figure 4



Testing at T0 - 50
Multiple Temperature Test Design
Testing at T0
Testing at T0 + 50
Average T0 Standard Error (Degrees C)
Sample Size
0
1
2
3
4
5
6
7
8
5
10
15
20
25

Figure 5



Lower Bound Coverage
Upper Bound Coverage
Interval Coverage
Sample Size
Sample Size
Sample Size

Figure 6

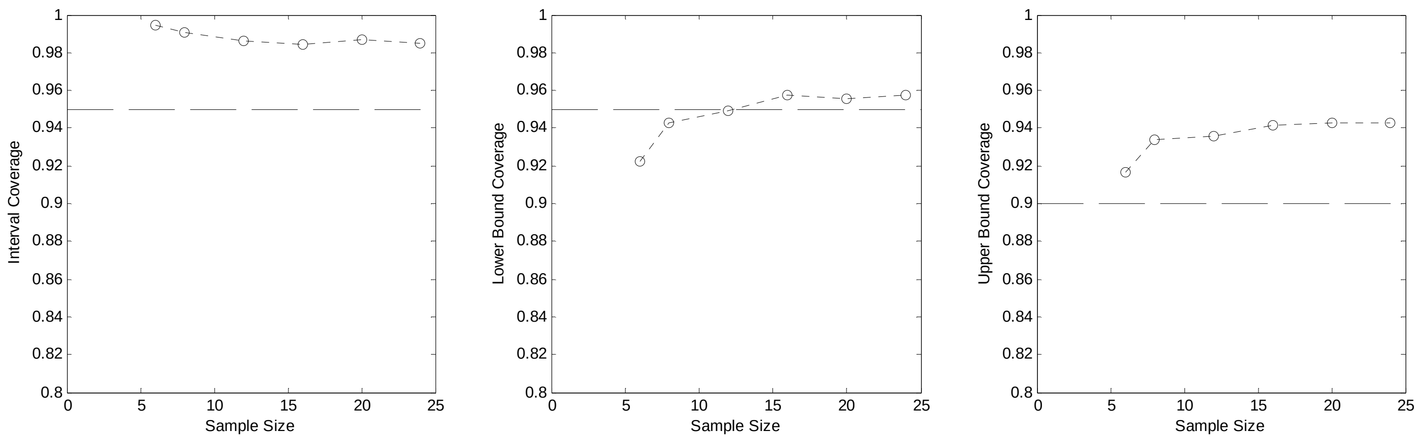

Interval Coverage
Sample Size
Lower Bound Coverage
Sample Size
Upper Bound Coverage
Sample Size
0.8
0.82
0.84
0.86
0.88
0.9
0.92
0.94
0.96
0.98
1
0
5
10
15
20
25

Figure 7

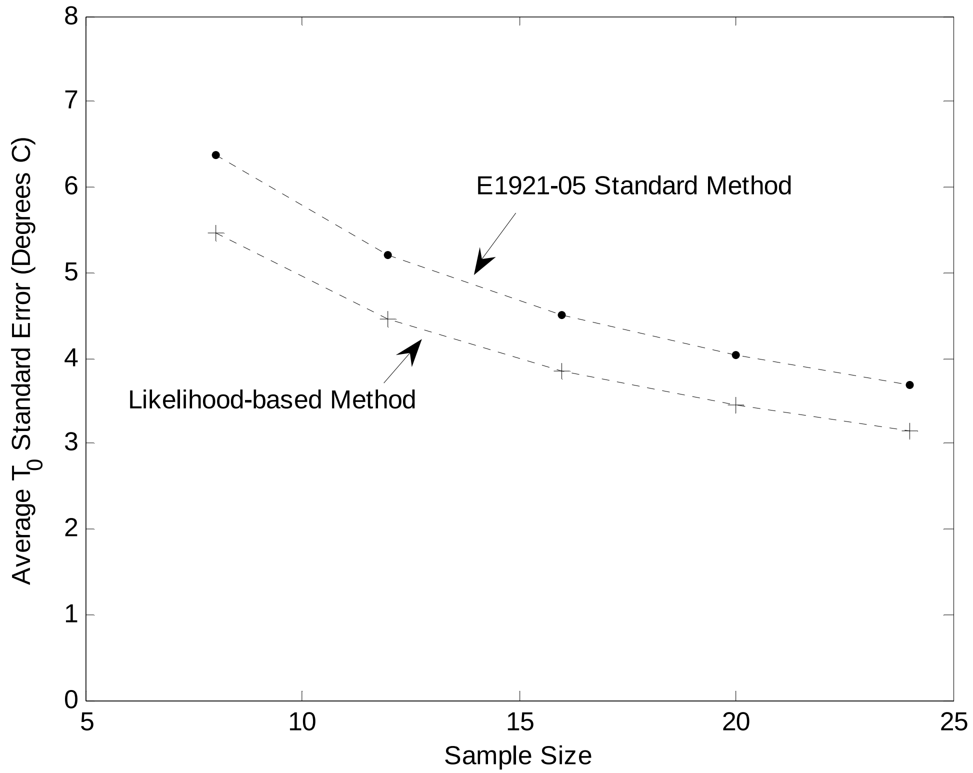

8
7
6
5
4
3
2
1
0
5
10
15
20
25
Average T_0 Standard Error (Degrees C)
Sample Size
E1921-05 Standard Method
Likelihood-based Method

Figure 8